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Aspen plus simulation of CO_2 removal from coal and gas fired power plants

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Abstract

This paper presents a description of the CO_2 removal process of 500MW coal and gas fired power plants. The parameters and other operating conditions for Aspen Plus rate based model were selected to achieve 85% of CO_2 removal. The effects of absorber pressure and packing height on re-boiler duty are studied. Re-boiler duty is decreasing with the increase of packing height and absorber pressure. The effect of solvent properties on CO_2 removal efficiency is also analyzed. The removal efficiency increases as the increase of MEA concentration and temperature. When the lean loading of MEA solvent is increased, efficiency of the removal process is decreasing. The liquid and vapour phase temperature profiles and CO_2 loading in the absorber are analyzed to understand the model behaviour.

Keywords: Carbon capture; Absorption; Aspen Plus; Sensitivity analysis; Re-boiler duty; Removal efficiency

1. Introduction

Carbon capture and storage (CCS) is considered as an important option for stabilization of atmospheric green house gases and minimizing global warming effects. Carbon dioxide (CO_2) is considered as the major green house gas, and fossil fuel fired power plants are the main emitting sources [1]. Therefore, the capture of CO_2 is important to maintain the emission levels according to the standards. There are three main options available for carbon capture in fossil fuel fired power plants: pre combustion CO_2 capture, where carbon is removed from the fuel prior to combustion; oxy-fuel combustion, where coal is combusted with oxygen instead of air with CO_2 enriched environment; and post combustion capture, where fossil fuel is combusted to produced energy and CO_2 is removed from the flue gas after combustion

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[2]. Out of these options, post combustion CO_2 capture by absorption and stripping process is currently considered as the most feasible option for CO_2 removal from fossil fuel fired power plants [3].

2. Model Development

The main problem of post combustion chemical absorption technology is the high installation cost and large amount of energy requirements in the re-generating sector. Therefore, the reduction of capital and operating cost are important to implement for the removal process in power plant flue gas treating. The model is developed and implemented in Aspen Plus to optimize the removal process. The Electrolyte NRTL (ELECNRTL) property method is used to handle the chemical reacting system in Aspen Plus. The flue gas streams data for 500 MW coal and gas fired power plant are extracted from the literature [1, 4]. The implemented process flow diagram is given in the Fig. 1.

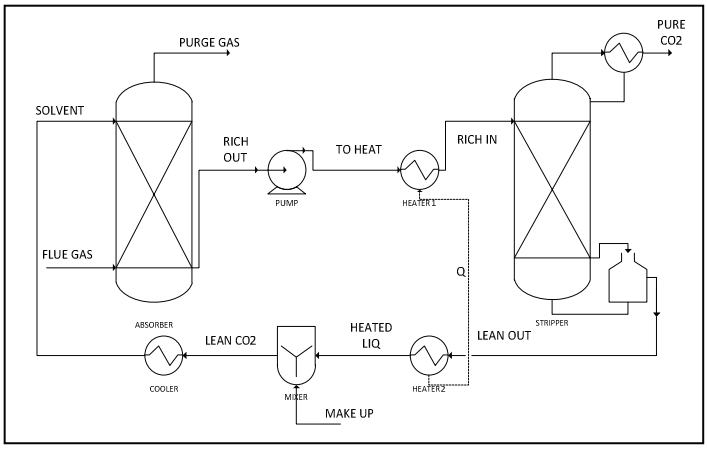

Fig. 1. Process Flow Diagram

In the chemical absorption, flue gas (FLUE GAS) enters the absorber at the bottom while the solvent (SOLVENT) enters at the top. The reactions start between MEA and CO_2 while flowing through the column (packing bed). An un-reacted gas leaves the column at the top (PURGE GAS), while the CO_2 rich solvent discharges the column at the bottom (RICH OUT). The rich solvent goes through the heat exchanger to increase the temperature before sending it to the stripper section. The heated rich MEA stream (RICH IN) then goes to the stripper at the top. In the stripper, steam is used for the regeneration process. Finally, separated acid gases leave the stripper at the top (PURE CO2). The lean MEA then leaves the system at the bottom of the stripper (LEAN OUT) and go through the heat exchanger. The MEA and water are added to the lean MEA stream (MAKE UP) to balance the component before recycled back to the absorber unit.

The flow diagram is modelled to capture the 85% of CO_2 from coal and gas fired power plants' flue gas with the variation of distillate rate in the stripper. Inlet flue gas and solvent stream are supplied at 40ºC and absorber is operating at 1bar absolute pressure. The rich solvent stream is heated up to 115ºC before sending it to the stripper section for maximum performance and the stripper is operating at 2 bars absolute pressure. The inlet flue gas stream data are given in the Table 1.

Table 1. Flue gas composition and parameters at inlet [1, 4]

Parameter	Coal Fired	Gas Fired
Flow rate [tones/hr]	2424	2861
Temperature [°C]	40	40
Pressure [bar]	1.1	1.1
Composition	Mol%	Mol%
H_2O	8.18	8.00
N_2	72.86	76.00
CO_2	13.58	4.00
O_2	3.54	12.00
H_2S	0.05	0.00

2.1. Chemical Reactions

The main chemical reactions taking place in a MEA+CO_2 system are described in this section. The absorption/stripping section required rigorous thermodynamic model [5] to find the equilibrium compositions in the system. Following chemical reactions (Equations 1-7) are taking place when CO_2 is absorbed into an aqueous solution [6].

Hydrolysis reaction:

$$MEACOO^- + H_2O \leftrightarrow MEA + HCO_3^- \quad (1)$$

Dissociation of dissolved carbon dioxide:

$$CO_2 + 2H_2O \leftrightarrow HCO_3^- + H_3O^+ \quad (2)$$

Dissociation of bicarbonate:

$$HCO_3^- + H_2O \leftrightarrow H_3O^+ + CO_3^{2-} \quad (3)$$

Dissociation of protonated MEA:

$$MEAH^+ + H_2O \leftrightarrow MEA + H_3O^+ \quad (4)$$

Ionization of water:

$$2H_2O \leftrightarrow OH^- + H_3O^+ \quad (5)$$

In addition to these main reactions, following two reactions are taking place when a sulphur compound exists in the flue gas system (coal fired flue gas).

Hydrogen sulfide:

$$H_2O + H_2S \leftrightarrow HS^- + H_3O^+ \quad (6)$$

Hydrogen bisulfide:

$$H_2O + HS^- \leftrightarrow S^{2-} + H_3O^+ \quad (7)$$

2.2. Equilibrium data

The mole fractions of every single component in the liquid and vapour phase are calculated by solving above equations. The equilibrium constant is calculated using following rate equation (equation 8).

$$\ln K_j = A_j + \frac{B_j}{T} + C_j \ln T + D_j T \quad (8)$$

The equilibrium constant data which is imported from Freguia [7] is considered for mathematical model development and tabulated in Table 2.

Table 2. Constant values of equilibrium constant equations [7]

Parameter	*Reaction 1*	*Reaction 2*	*Reaction 3*	*Reaction 4*	*Reaction 5*	*Reaction 6*	*Reaction7*
A_j	-0.52	231.46	216.05	-3.038	132.89	214.58	-9.74
B_j	-2545.53	-12092.1	-12431.7	-7008.3	-13445.9	-12995.4	-8585.47
C_j	0	-36.78	-35.48	0	-22.47	-33.55	0
D_j	0	0	0	-0.00313	0	0	0

2.3. Rate kinetic data

Rate kinetic data are important to understand for reacting system. The equilibrium reactions 1 and 2 are replaced by rate model equations 9 and 10 and reverse reactions 11 and 12.

$$CO_2 + OH^- \rightarrow HCO_3^- \quad (9)$$

$$MEA + CO_2 + H_2O \rightarrow MEACOO^- + H_3O^+ \quad (10)$$

$$HCO_3^- \rightarrow CO_2 + OH^- \quad (11)$$

$$MEACOO^- + H_3O^+ \rightarrow MEA + CO_2 + H_2O \quad (12)$$

The kinetic equation used for mathematical calculations is defined in Aspen Plus and given in Equation (13) with constant values in Table 3.

$$r_j = k_j \left(\frac{T}{T_O}\right)^{n_j} \exp\left[-\frac{E_j}{R}\left(\frac{1}{T} - \frac{1}{T_O}\right)\right] \quad (13)$$

Table 3: Rate constant values

Parameter	*Reaction 9*	*Reaction 10*	*Reaction 11*	*Reaction 12*
k_j	4.32e+13	9.77e+10	2.38e+17	2.7963e+20
n_j	0	0	0	0
E_j (cal/mol)	13249	9855.80	29450.89	17229.79
T_O (K)	298	298	298	298

3. Simulations

The main idea of this paper is to develop the model that will help to optimize the process with sensitivity analysis. Initially, the open loop process flow diagram is developed to optimize the parameters and finally, the process flow diagram is modified with optimized parameters for closed loop system. Open loop model should be used for parameter optimization. Once the process flow diagram is closed, model is not able to use for parameter optimization due to recirculation stream. The process model is closed with individual material balance. Therefore, change of one parameter causes to change the material balance in the process.

3.1. Solvent properties effect on removal efficiency

The sensitivity analysis is performed to check the solvent properties' behaviour for removal efficiency in capture plant. As the most important factors, solvent strength, lean loading and solvent temperature are considered for analyzing. According to the variation of these factors, removal efficiency is studied and given in Fig. 2-4, respectively.

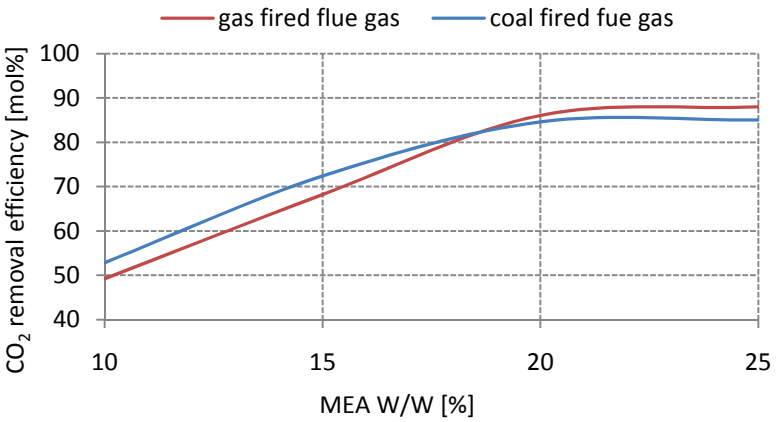

Fig. 2. CO_2 removal efficiency variation with MEA concentration

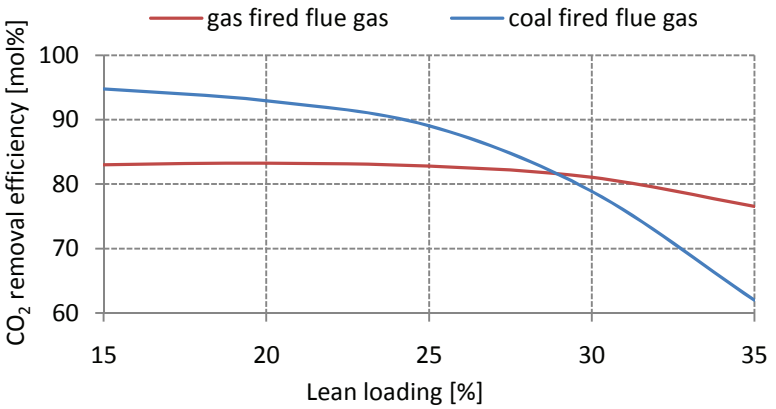

Fig. 3. CO_2 removal efficiency variation with lean loading

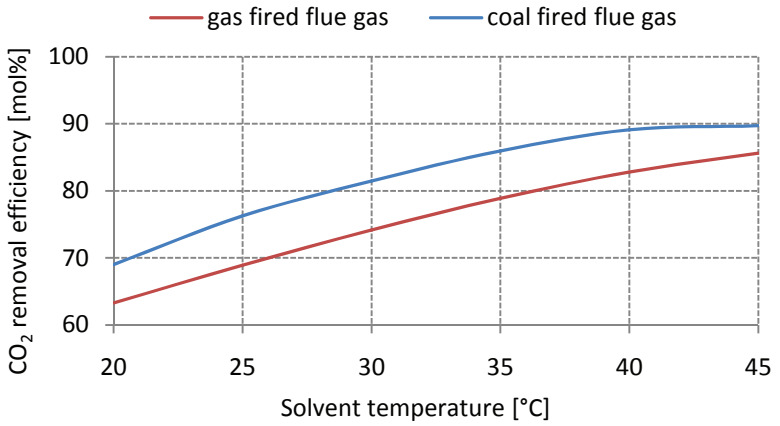

Fig. 4. CO_2 removal efficiency variation with solvent temperature

As it can be seen from Fig. 2 and 4, the efficiency of the CO_2 removal is increased as the MEA strength and solvent temperature are increased. The maximum efficiency is achieved when MEA concentration at 22-25% and temperature is around 40-45°C. When the lean loading of MEA solvent is increased, efficiency of the removal process is decreasing (Fig. 3). Both gas and coal fired flue gas system follow the similar pattern in all three cases. However, the values of coal fired flue gas model are slightly higher than the gas fired model.

3.2. Parameters effect on re-boiler duty

The main problem with the post combustion capture is the high energy requirement in the regeneration sector, i.e. re-boiler duty in stripper column. Therefore, parameters' effect on the re-boiler duty is important to optimize. The effect of absorber pressure and absorber packing height on re-boiler duty is studied to optimize the energy requirement. Fig. 5 and 6 represent the re-boiler duty variation with absorber pressure and packing height, respectively. With the increase of absorber pressure and packing height, re-boiler duty is decreased. Gas fired flue gas system has higher re-boiler duty compared to the coal fired system. Reason for that is, gas fired flue gas consist of fewer carbon dioxide amounts compared to coal fired flue gas. Therefore, to achieve the same efficiency defined in the model is required to process more flue gas compared to the coal fired system.

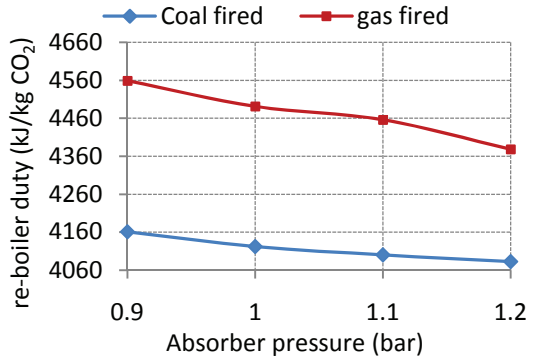

Fig. 5. Re-boiler duty variation with Absorber pressure

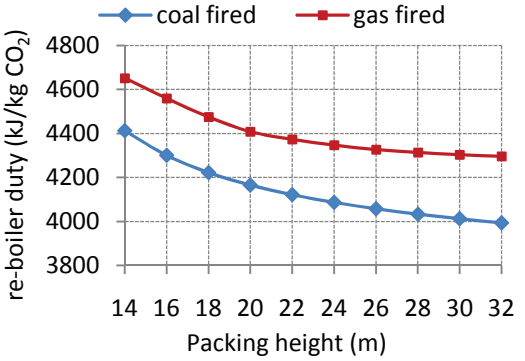

Fig. 6. Re-boiler duty variation with absorber packing height

3.3. Simulated profiles for closed loop capture model

The process flow diagram is implemented with the optimized parameters for closed loop system. After the simulation, temperature profiles, CO_2 concentration profiles and loading are analyzed for both coal and gas fired implemented model to understand the model behaviour. Fig. 7 represents the liquid and vapor phase temperature profiles in the absorber for coal and gas fired systems. According to the Fig. 7, the coal fired flue gas model has higher temperature range along the column. Coal fired flue gas consist of more CO_2 than gas fired system. Therefore, more reactions are taking place in the absorber column in coal fired model. Hence, liquid and vapour phase temperature of the absorber unit are increasing and maximum value is higher in gas fired system temperature profiles. The temperature profiles in both liquid and vapour phases are overlapped in gas fired system and slight deviation in coal fired process. Similarly,

Fig. 8 represents the liquid phase CO_2 loading in the absorber. The CO_2 loading is gradually increasing down the column for both cases.

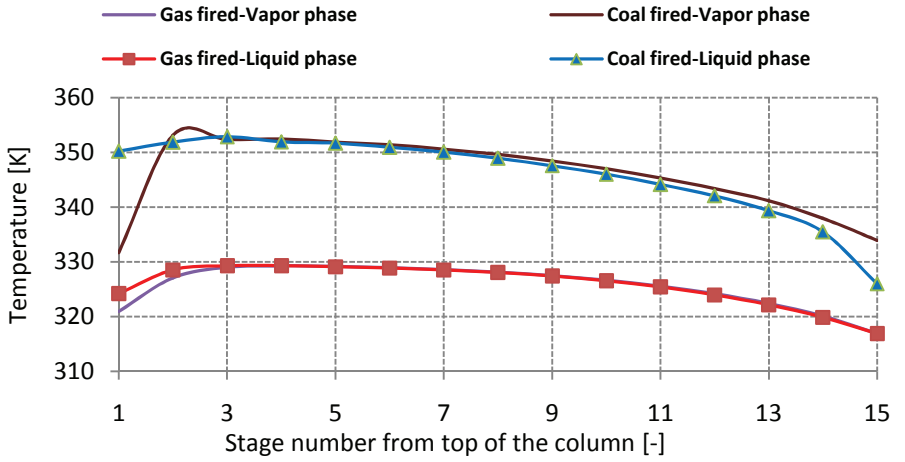

Fig. 7. Liquid and vapor phase temperature profiles in absorber

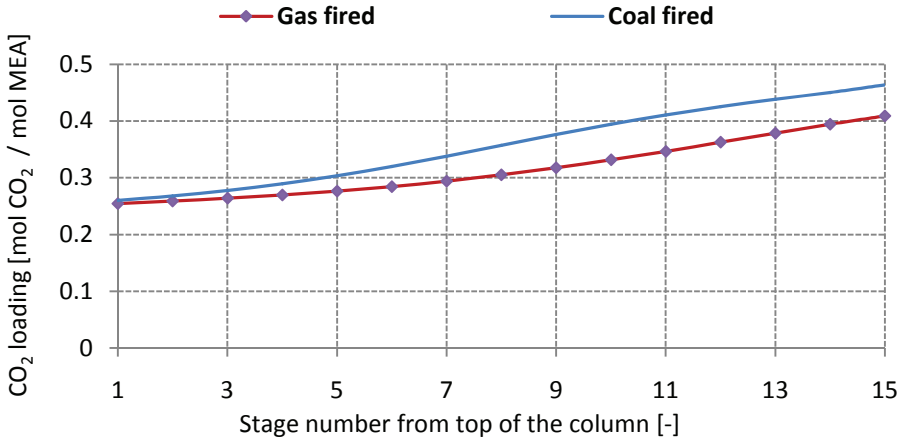

Fig. 8. CO_2 loading in absorber

4. Discussion and Conclusion

The efficiency of the removal process is strongly depending on the solvent properties like solvent concentration, lean loading and solvent temperature. The removal efficiency is proportional to the solvent concentration and temperature while lean loading is inversely effect on removal efficiency. This is because of; increasing the amine concentration will cause for the increasing capture capacity. With the increase of lean loading, the capacity of the solvent for CO_2 absorption decreases, hence efficiency of the CO_2 removal is decreasing. As the solvent temperature increases, the driving force for absorption

decreases. However, the rate of reaction and diffusivity increases as the solvent temperature is increased. Therefore, efficiency of CO_2 removal is increased with the increase of solvent temperature.

The re-boiler duty is functions of absorber pressure and absorber packing height and when the increase of both factors, re-boiler duty is decreased. The reason for that is the attained rich loading increase with the increases in the absorber packing height. Similarly, re-boiler duty decreases with the increase of absorber pressure due to higher CO_2 partial pressure. The required re-boiler duty was calculated as 4540 kJ/kg CO_2 for the gas fired flue gas system and 4100 kJ/kg CO_2 for coal fired flue gas system. Both re-boiler duties are reasonable with the literature values [3].

The implemented model in Aspen Plus for gas and coal fired removal system functioned properly. The amount of CO_2 removal is 85% and calculated with the variation of distillate rate in the stripper. The make up stream is added to maintain the component losses during the process. The MEA and H_2O requirement for the make-up stream was calculated as 362 kg/hr and 87.8 tones/hr for gas fired system and 627 kg/hr and 119 tones/hr for coal fired system, respectively.

Both temperature profiles in liquid and vapor phase follow the similar patterns and temperature bulges are shown close to top of the column. Coal fired temperature profile reach higher temperatures than gas fired system. The CO_2 loading profile has the similar flow pattern in both cases. The maximum value is reached to around 0.4 and higher in coal fired flue gas system. Those profiles are important to understand the column behaviour.

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